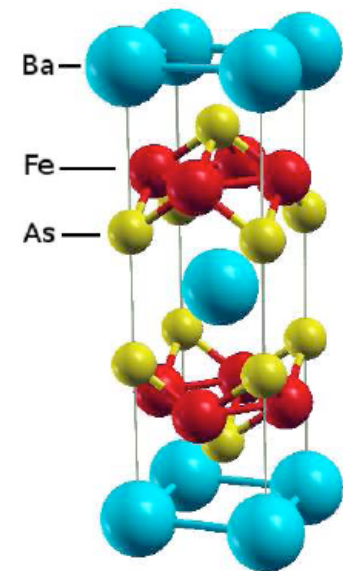
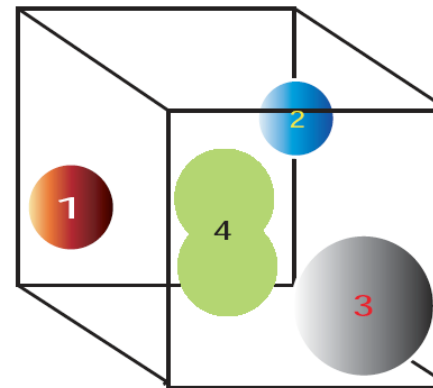
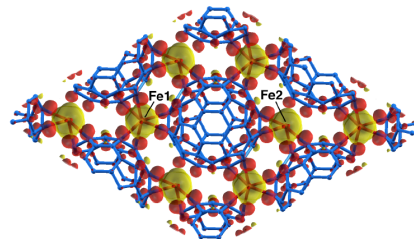
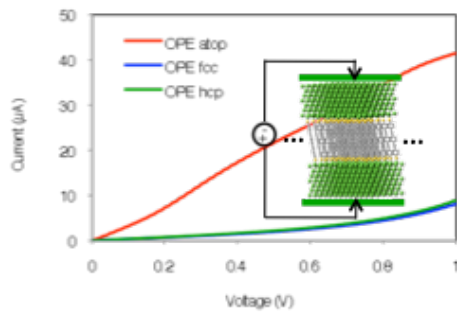
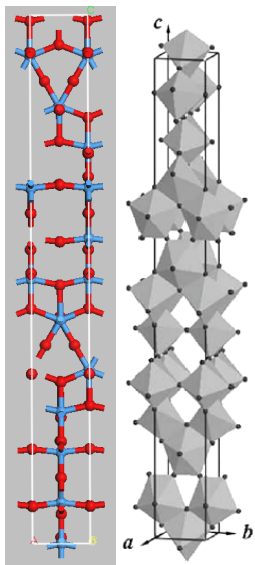
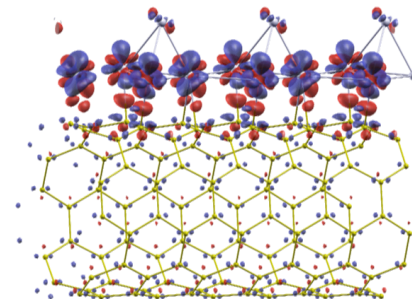


Simulation based on DFT

Hai-Ping Cheng, Dept. of Physics and the Quantum Theory Project, University of Florida



UF-HPC



Theoretical Methods

- First-Principles calculations based on density functional theory
- Green's function techniques
- Molecular Dynamics
- Boltzmann equation
- Beyond LDA-GGA (+U, QMC, GW...)
- Multi-scale Simulations

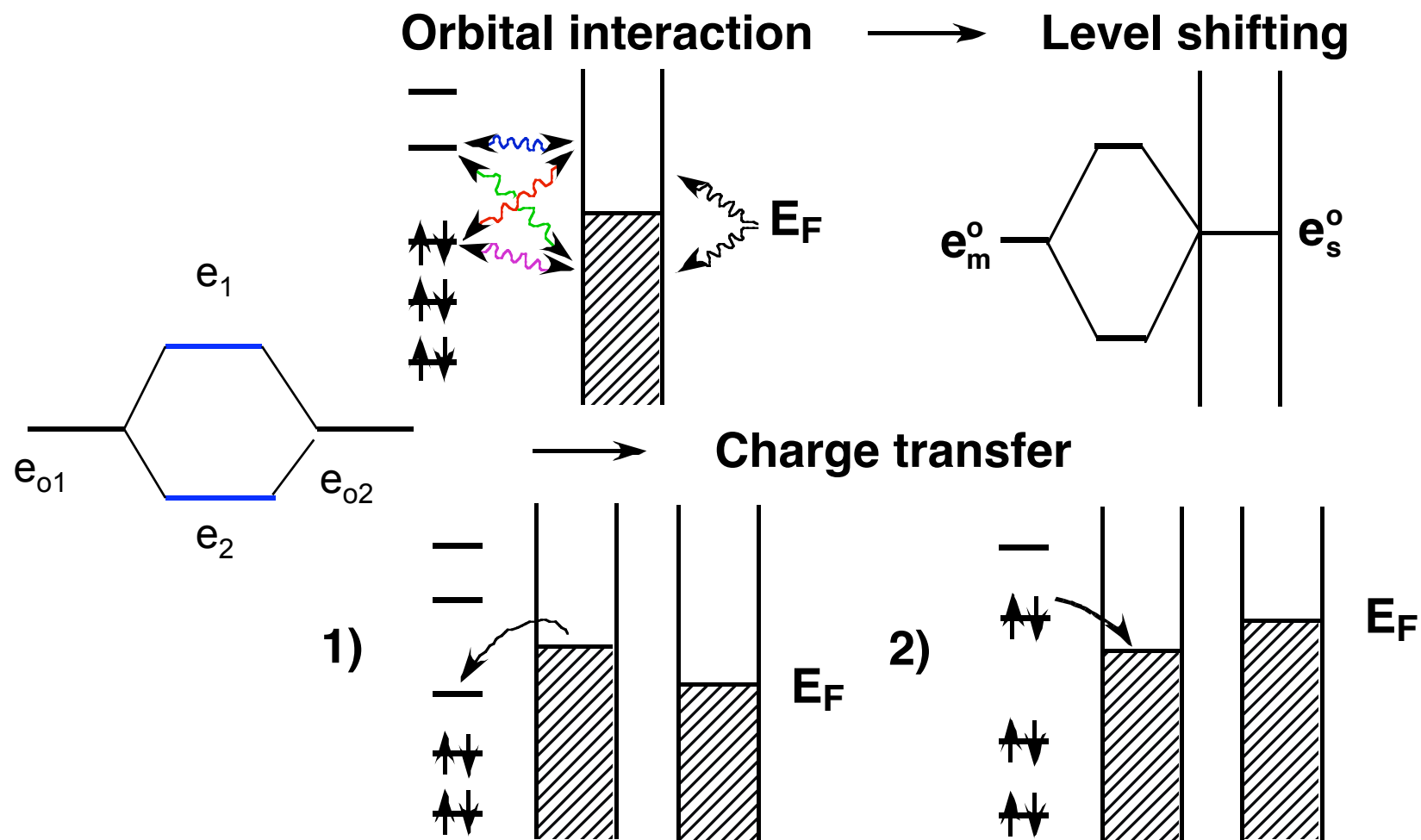
Computer Software

- PWSCF, VASP, BO-LSD-MD, SIESTA
- SMEAGOL, Igator, Layer KKR, PWSCF-Cond
- DL_POLY, AMBER
- Boltzmann transport (no-name)
- CASINO, SAX, SAX-Spin
- OPAL: Multi-scale Simulations

Approach Scientific Problems via computational physics

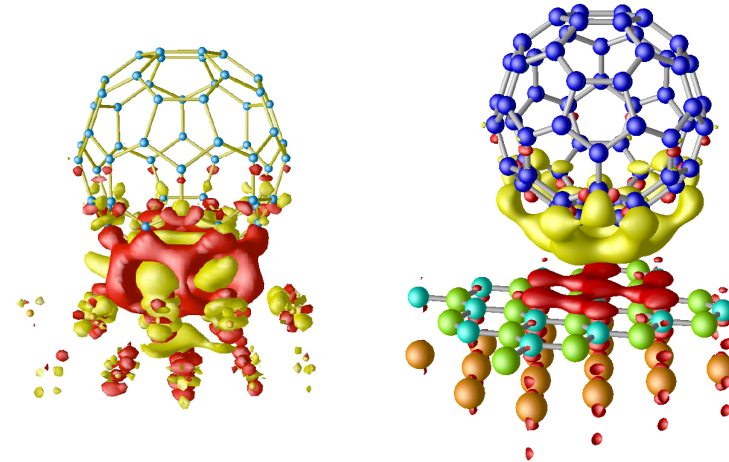
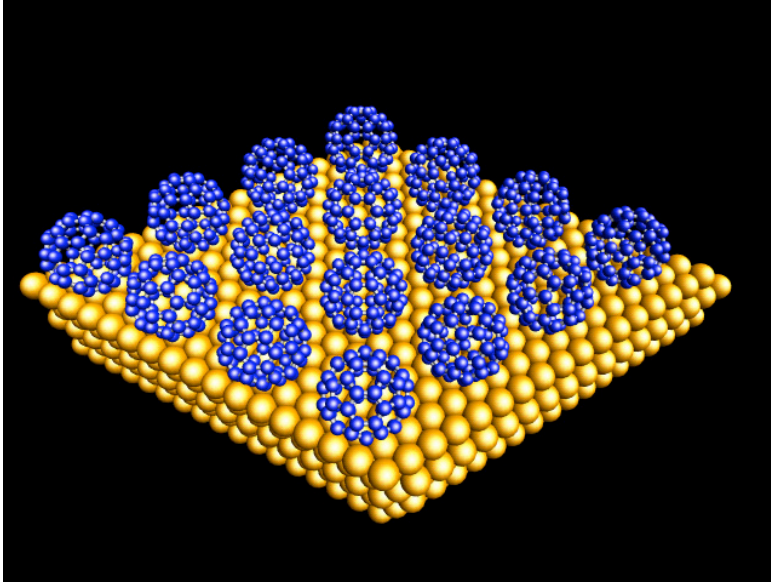
- Particle surface interaction: structure, dynamics, charge transfer, magnetic pattern
- Transport: Coherent vs. diffusive, interplay between conductance and structure, spin, chemical doping, external field.
- Hydrolytical weakening of materials: Bond weakening due to interaction with water, complex materials (e.g. Bone)
- High T_c materials, materials for optical coating (phonon-electron coupling, phonon spectrum)

Molecule-surface interaction



C_{60} on surface

Li, Wu, and Cheng, JCP (2010)
Che and Cheng, PRB (2005)
Wang and Cheng PRB (2004)



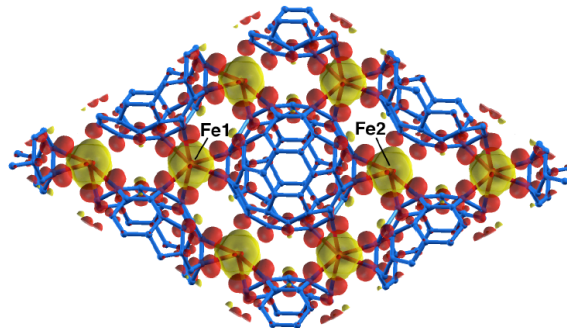
Red: hole and yellow: electron. Left: C_{60} on Cu; right: C_{60} on BN/Ni(111). Charge transfer to C_{60} does not always give surface dipoles with the same sign.

Done: ~2000 electrons

Plan (if resource is available): ~10,000 electrons
to include surface reconstruction etc.

Fe-doped C_{60} on
surface

Yellow: spin up and
red down

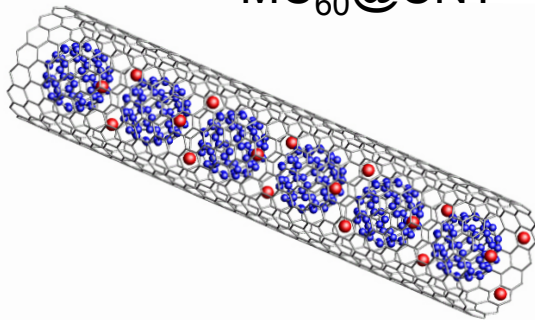


	Fe				C_{60}		
	<i>s</i>	<i>p</i>	<i>d</i>	$m_{Fe}(\mu_B)$	<i>s</i>	<i>p</i>	$m_{C60}(\mu_B)$
FeC ₆₀ /h-BN/Ni							
GGA	↑0.01	↑0.01	↑2.42	+2.45	↓0.01	↓0.35	-0.37
LDA	↑0.04	↑0.01	↑1.92	+1.96	↓0.01	↓0.38	-0.38
Fe ₂ C ₆₀ /h-BN/Ni							
GGA	↑0.03	↑0.02	↑4.66	+4.71	↓0.03	↓0.68	-0.71
LDA	↑0.07	↑0.01	↑3.38	+3.46	↓0.03	↓0.67	-0.70
Fe ₃ C ₆₀ /h-BN/Ni							
GGA	↑0.03	↑0.03	↑6.76	+6.82	↓0.04	↓0.71	-0.76
LDA	↑0.03	↑0.03	↑6.40	+6.46	↓0.02	↓0.60	-0.63
Fe ₄ C ₆₀ /h-BN/Ni							
GGA	↑0.04	↑0.03	↑9.14	+9.21	↓0.04	↓0.66	-0.70
LDA	↑0.03	↑0.05	↑8.74	+8.82	↓0.03	↓0.55	-0.58
GGA + U	↑0.02	↑0.01	↑11.00	+11.03	↓0.04	↓0.48	-0.52
LDA+U	↑0.01	↑0.01	↑10.75	+10.77	↓0.03	↓0.51	-0.54
Fe ₁₅ C ₆₀ /h-BN/Ni							
GGA	↑0.02	↓0.13	↑29.47	+29.36	↓0.05	↓0.53	-0.58
LDA	↓0.02	↑0.02	↑24.29	+24.29	↓0.03	↓0.49	-0.51
GGA+U	↑0.08	↓0.01	↑38.80	+38.87	↓0.06	↓0.49	-0.54
LDA+U	↓0.05	↓0.11	↑30.70	+30.54	↓0.05	↓0.62	-0.66

M_n - C_{60} doped peapods

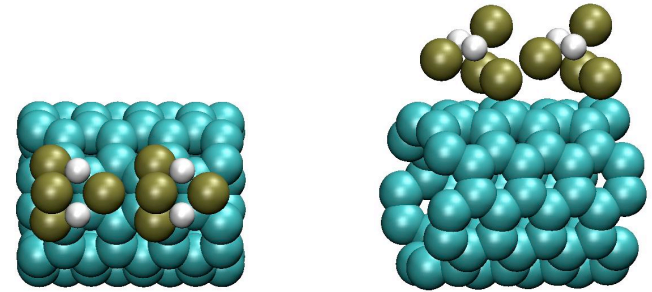
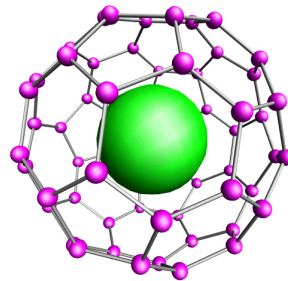
H_2 dissociation on Pd_4 coated CNT

$MC_{60}@CNT$

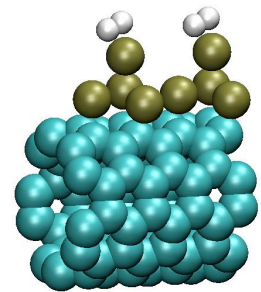
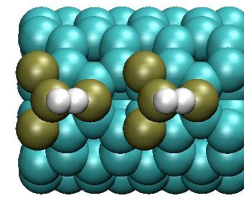


Du and Cheng, PRB (2004)

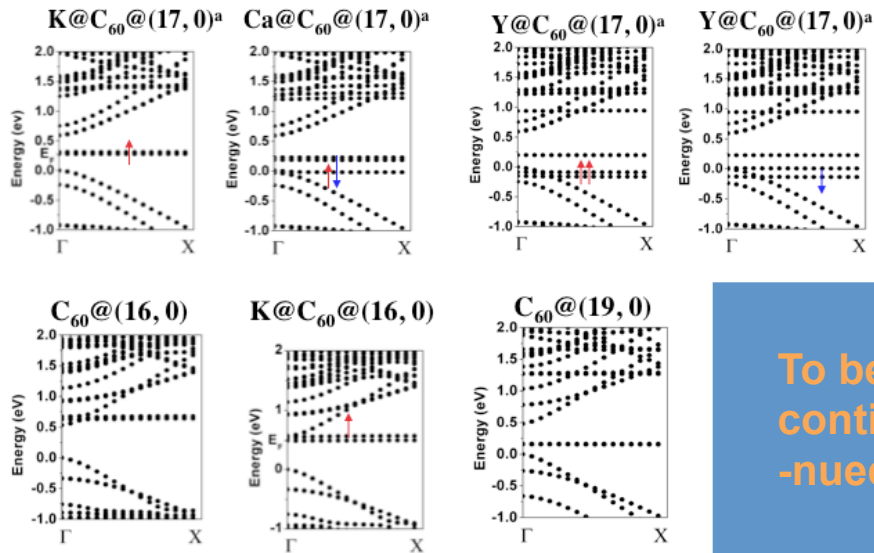
$M@C_{60}$



Cao and Cheng (2009)

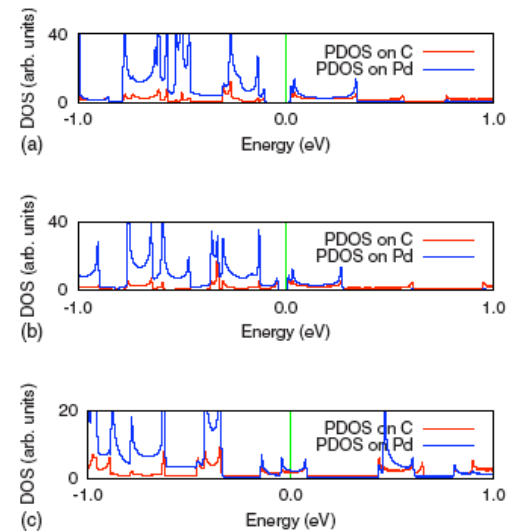


Band Engineering via doping

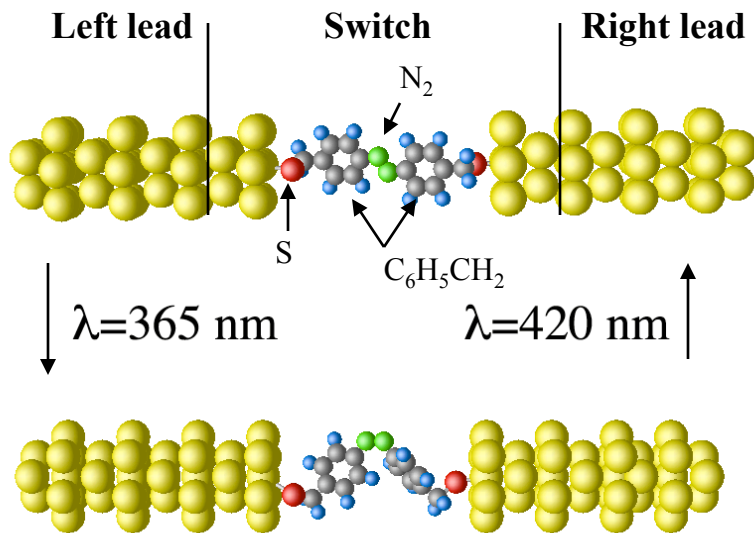


To be
conti
-nued

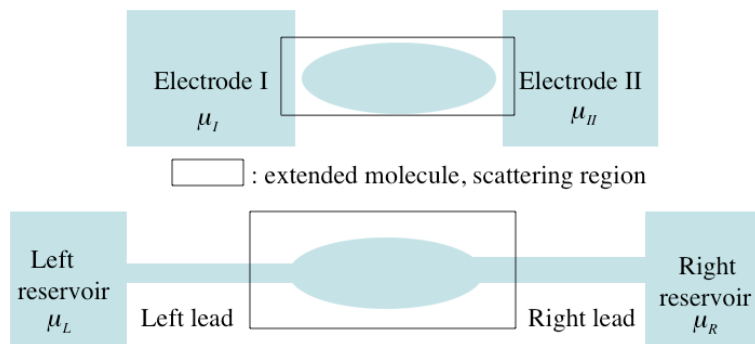
Reaction induced band structure change



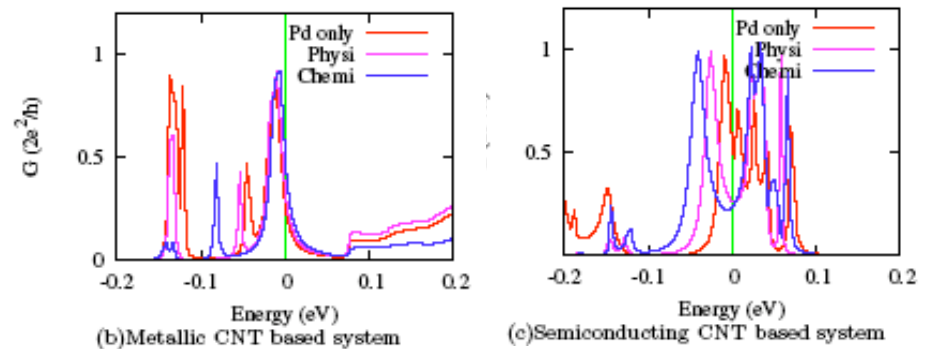
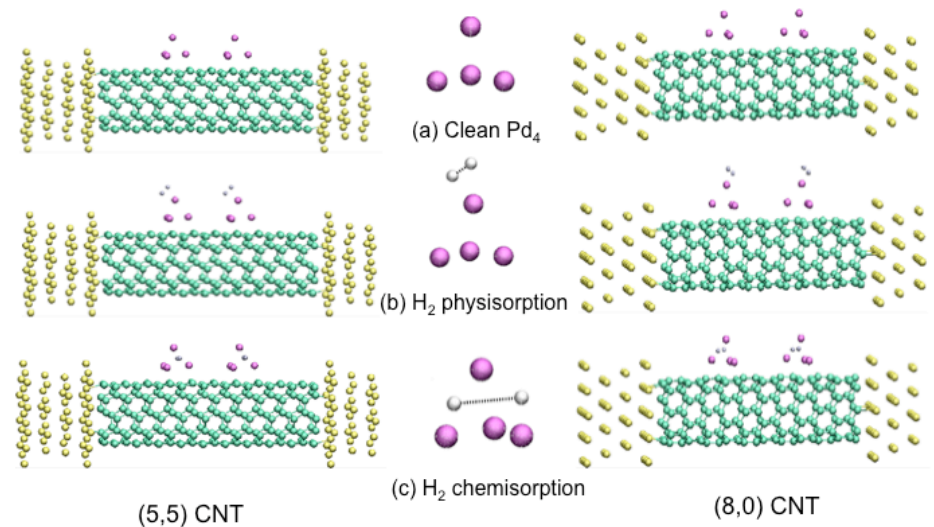
Electron Transport



Light-induced switching in azobenzene crans: on state, cis: off state



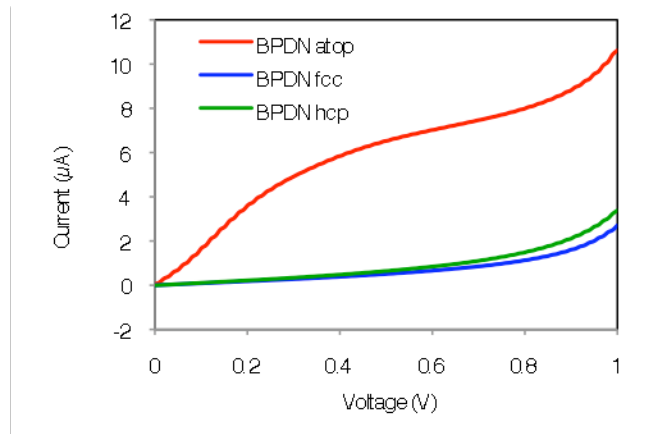
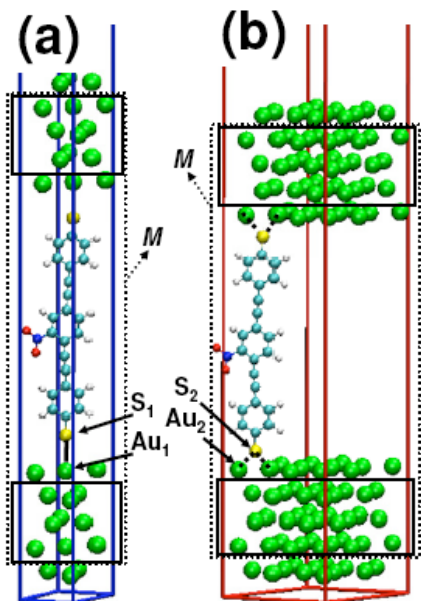
Zhang et al (2004)



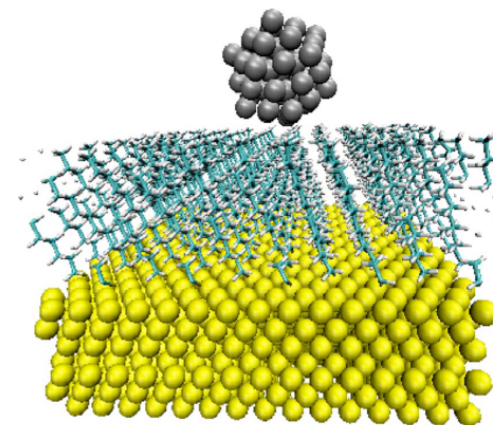
Metallic and semiconductor CNTs are both good at probing H₂, but they work in opposite direction.

Cao et al (2009)

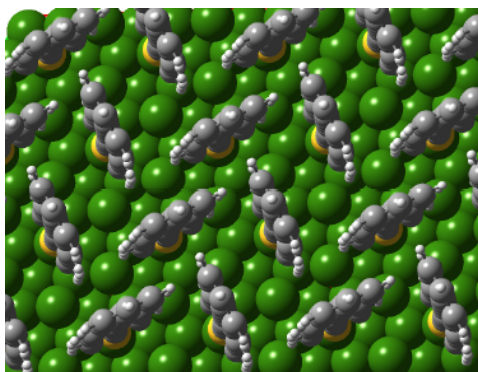
2D transport: SAMs dynamics, transport



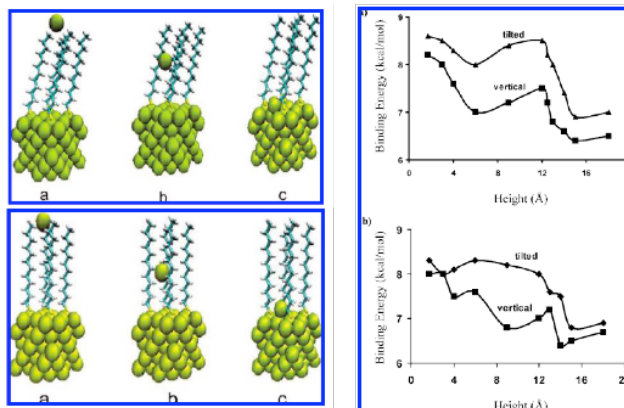
Site-sensitive conductance
Agapito and Cheng (2009)



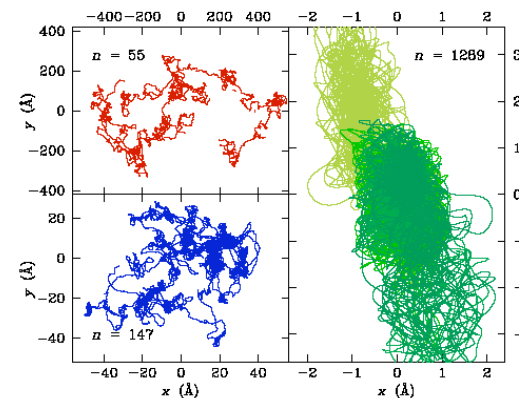
Size dependent Ag_n
diffusion on SAM/gold
Alkis et al (2009)



Top view: Herringbone
structure

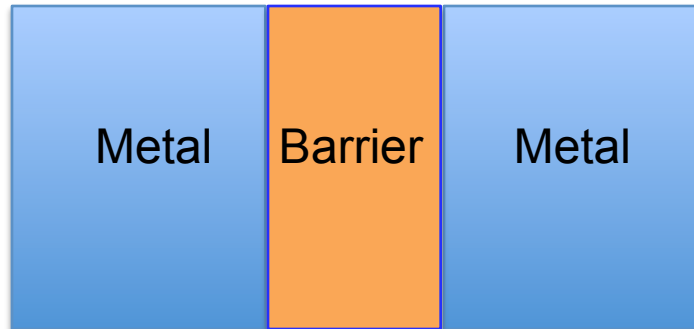


Au penetration through SAM molecules

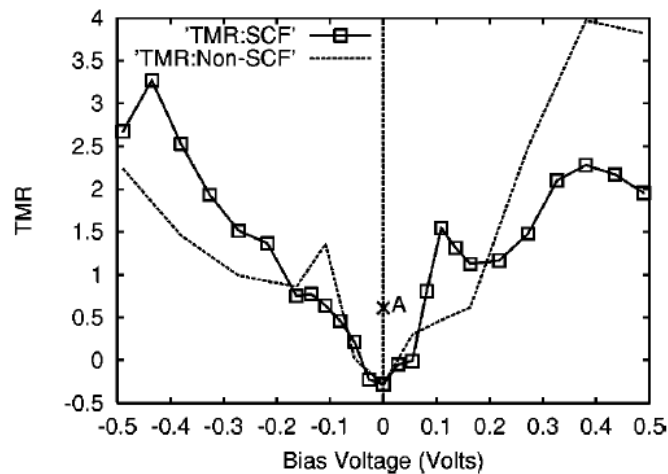


Spin-dependent transport of MgO magnetic tunnel junctions

spin-dependent tunneling under a finite bias

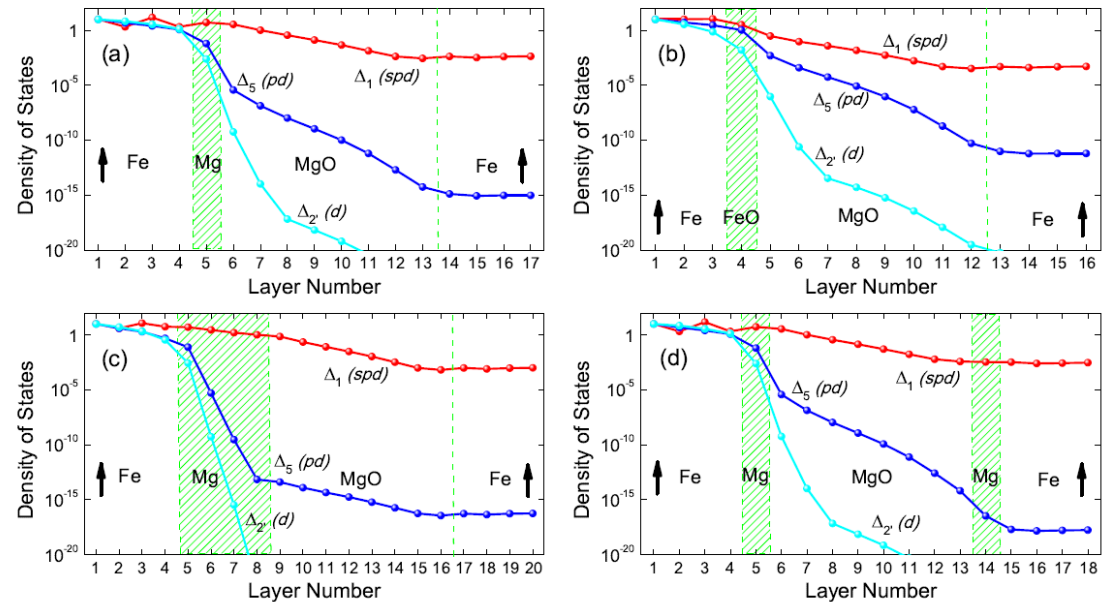
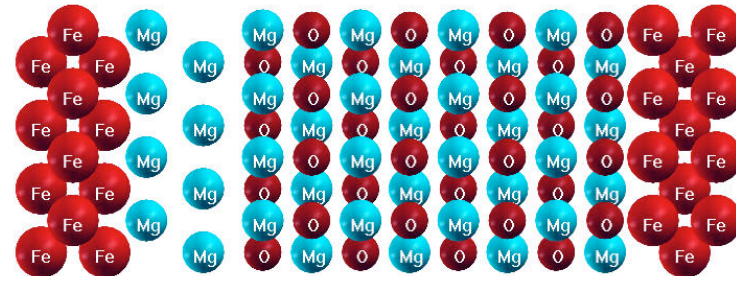


Spin-polarized self-consistent DFT method for calculation of the electronic structure and transport properties of a system under a finite bias voltage, implemented within the Layer-KKR approach.



C. Zhang, *et. al.*, PRB (2004)

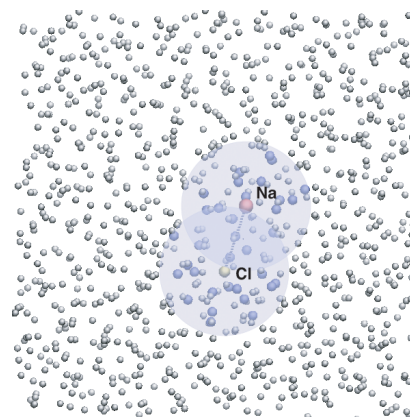
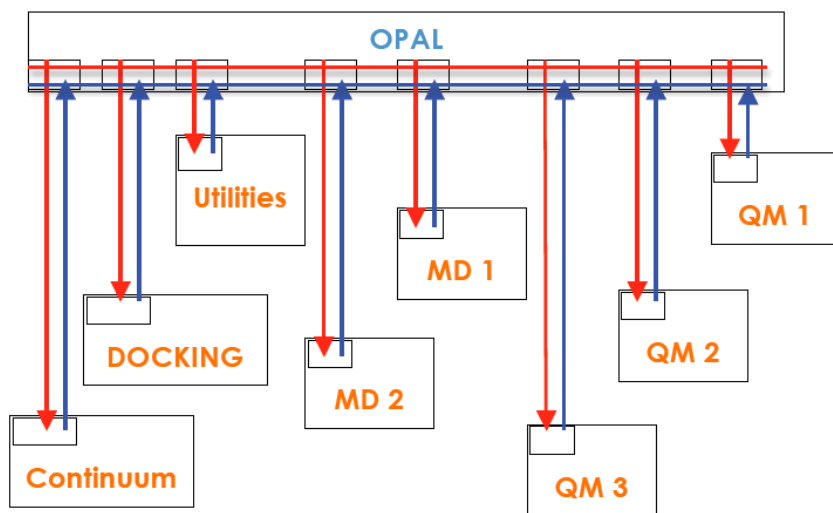
Role of Mg interlayer in Fe/Mg/MgO/Fe junctions



Tunneling density of states for
(a) Fe/Mg(1)/MgO/Fe; (b) Fe/FeO(1)/MgO/Fe-
(c) Fe/Mg(4)/MgO/Fe; (d) Fe/Mg(1)/MgO/Mg(1)/Fe-

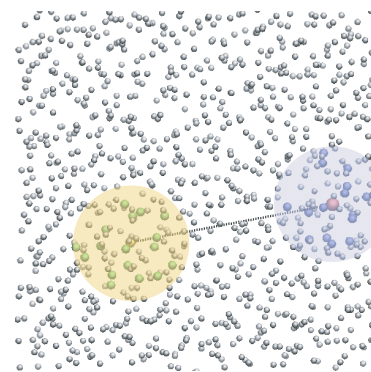
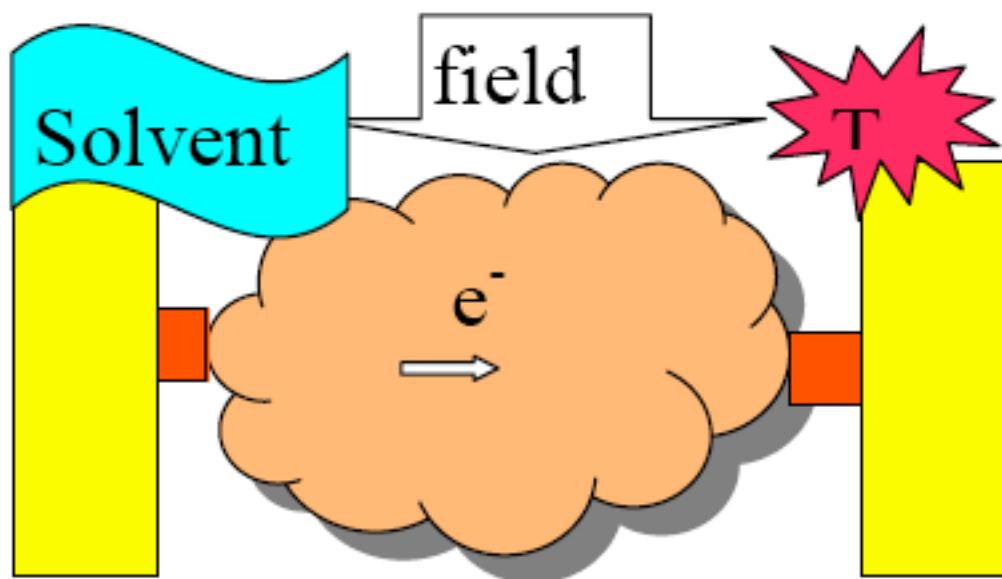
Y. Wang, *et. al.*, to be submitted (2010).

OPAL: A MPI-2 based multi-scale simulation architect



Before: 1 Q-region
Run 1 SIESTA

Optimistic scenario:
Each quantum subregion
Contains 100-1000 atoms
Linear scaling on 1000
cpu, run 1000 copies of
DFT code that describes
1000 quantum subregions.
Atomistic MD code will
treat 10^6 - 10^8 atoms and
fluid dynamics description
can also be used when
necessary.



After: 2-Q region
Run 2 SIESTA and 1
DL_POLY independ-
ently

Current and 5-year projection

Machines used--

NERSC HOPPER, Franklin, Jaguar, BASSI,

VASP, PWSCF, SIESTA, SMEAGOL, TranSiesta:

UF/HPC Clusters; NERSC Franklin, Hopper, Jaguar;

DL_POLY, iGator: UF/HPC Clusters

cores, amount of memory, input/output, disk storage
typically used

VASP: (see Stocks' talk)

PWSCF Cores: 10^2 : Memory ~2GB/core; I/O and disk no severe limitations

SIESTA, SMEAGOL, TranSiesta Cores: 10: Memory ~2GB/core

DL_POLY: Cores: 10 - 10^2 Memory ~1GB/core

Required libraries: scalapack, blas

iGator needs parallel MATLAB

Most severe limitation is maximal CPU time on NERSC machine, 24-48 hours,
7x24 hours is sometime need and 72 hours is often needed.

Wish list –

Much more allocation – finite temperature first-principles statistical physics

Short waiting time to access > 128 cpu

Long cpu time limit

Opportunity to test OPAL with 1000 quantum regions using 1,000-10,000 CPU

Assistance to fully optimize PWSCF and VASP (as Paul Kent did for VASP)